An Adaptive Chemistry Approach to Modeling Emissions Performance of Gas Turbine Combustors, Phase II

Completed Technology Project (2009 - 2011)

Project Introduction

Computational Fluid Dynamics (CFD) simulations for combustion do not currently have the predictive capability typically found for non-reacting flows due to the prohibitively high computational cost incurred when one introduces detailed chemical kinetics. In this SBIR project, we propose a novel method, Adaptive Chemistry, to enable such detailed modeling. This method adapts the reaction mechanism used in CFD to local reaction conditions. Instead of a single comprehensive reaction mechanism throughout the computation, smaller, locally valid reduced models are used to accurately capture the chemical kinetics at a smaller cost. Our Adaptive Chemistry approach seeks to obtain a reduced model guaranteed to be valid within the variable range for each grid point, and controls errors rigorously without evaluating the very expensive full model. Adaptive Chemistry also dynamically constructs a reduced model library based on real-time reaction conditions to prevent large memory overhead for arbitrary solution trajectories. This also allows Adaptive Chemistry to be easily extendable to transient problems. Finally, Adaptive Chemistry allows users to set a constraint on the largest model size by using a skeletal model, but selects each reduced model based on the full, detailed chemistry, which obtains a guaranteed optimal solution more efficiently compared to the traditional skeletal model methods. In this project, we will develop an error-controlled reduced-species Adaptive Chemistry software package that can be easily interfaced with any CFD solver. The first objective of this work is to continue developing needed methods for error-controlled reduced-species Adaptive Chemistry for steady-state reacting flow simulations. The second objective is to implement the available methods into a modular package that can be easily interfaced with any CFD solver. We will also develop an Adaptive Chemistry module that can be coupled with the PREMIX program for commercialization.

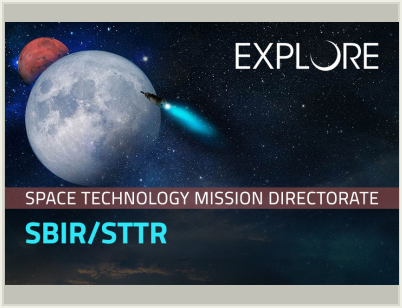

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Table of Contents

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Center / Facility:

Glenn Research Center (GRC)

Responsible Program:

Small Business Innovation Research/Small Business Tech Transfer

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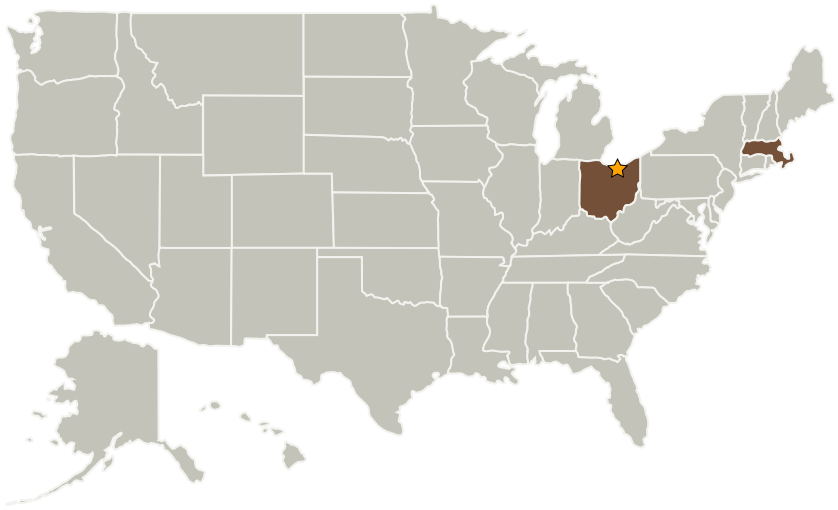
Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
★Glenn Research Center(GRC)	Lead Organization	NASA Center	Cleveland, Ohio
Aerodyne Research, Inc	Supporting Organization	Industry	Billerica, Massachusetts

Primary U.S. Work Locations	
Massachusetts	Ohio

Project Transitions

December 2009: Project Start

June 2011: Closed out

Project Management

Program Director:

Jason L Kessler

Program Manager:

Carlos Torrez

Technology Areas

Primary:

- TX15 Flight Vehicle Systems
  - TX15.1 Aerosciences
    - TX15.1.7 Computational Fluid Dynamics (CFD) Technologies